2H-THIOPYRAN-3-CARBOXALDEHYDE, 5,6-DIHYDRO-2,6-DIMETHYL-

Other names: 2,6-Dimethyl-5,6-dihydro-2H-thiopyran-3-carbaldehyde
Inchi: InChI=1S/C8H12OS/c1-6-3-4-8(5-9)7(2)10-6/h4-7H,3H2,1-2H3
InchiKey: OVGLVUDQBOCQPR-UHFFFAOYSA-N
Formula: C8H12OS
SMILES: CC1CC=C(C=O)C(C)S1
Mol. weight [g/mol]: 156.25

Physical Properties

Property code	Value	Unit	Source
hfus	16.16	kJ/mol	Joback Method
logp	2.026		Crippen Method
mcvol	126.340	ml/mol	McGowan Method
rinpol	1240.00		NIST Webbook
rinpol	1240.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.04	J/mol×K	497.95	Joback Method
cpg	285.76	J/mol×K	535.42	Joback Method
cpg	299.67	J/mol×K	572.90	Joback Method
cpg	312.80	J/mol×K	610.37	Joback Method
cpg	325.15	J/mol×K	647.84	Joback Method
cpg	336.75	J/mol×K	685.32	Joback Method
cpg	347.61	J/mol×K	722.79	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13643964&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices